

Summary

This work investigates the properties of nitrogen and phosphorous encapsulated in the Buckminster–fullerene C_{60} for an application as qubits in a quantum computer.

Previous works proved the existence of group V endohedral fullerenes. The (cw) ESR spectra showed sharp resonance lines even for chemical modifications of $N@C_{60}$. First relaxation measurements of $N@C_{60}$ indicated that these endohedral fullerenes might be good candidates for qubits in a quantum computer. This idea has been developed systematically in this thesis.

In this work, it has been shown for the first time that the separation and enrichment via HPLC is possible for $P@C_{60}$. The first intensive investigation of the spectroscopic properties of $P@C_{60}$ has been done and consequences of the results for quantum computing with endohedral fullerenes have been discussed.

The relaxation properties of $P@C_{60}$ have been examined in detail. It has been shown that they are similar to those of $N@C_{60}$. The model for relaxation has been reviewed and improved evaluating the limits of the harmonic oscillator model. The relaxation properties remain mainly molecular even if the spin concentration increases. This means that a quantum computer using endohedral fullerenes might be scalable towards numerous qubits if the dipolar coupling between them is controlled.

More spectroscopic properties of $P@C_{60}$, especially the zero–field splitting that could not be resolved so far, have been investigated using transient nutation experiments. This method has been applied to endohedral fullerenes for the first time. For a quantum computer, transient nutation reveals the behaviour of the spin system under single qubit operations. It has been shown for $N@C_{60}$ and $P@C_{60}$ that numerous operations can be done at room temperature.

Low temperature measurements showed that the nutation of a $S = 3/2$ system is complicated under special conditions. The experiments reveal nutation frequencies as predicted by theory. It seems to be possible to implement two qubits in one spin with $S = 3/2$. However, an alignment of the molecules would be necessary in this case. At the same time, such an alignment would provide control over the dipolar interaction.

Therefore, in the last part of this thesis the orientation of endohedral fullerenes in a liquid crystal matrix has been investigated. It has been shown that the alignment of the endohedral monomers $N@C_{60}$ and $N@C_{70}$ is possible. However, the alignment of larger molecules like dimers is more difficult although initial steps could be demonstrated.

If full orientation of endohedral fullerenes can be achieved while keeping a well–defined distance between them, quantum computing with group V endohedral fullerenes seems to be feasible.